Spin susceptibility and the π-excitation in underdoped cuprates.

Jan Brinckmann and Patrick A. Lee
Massachusetts Institute of Technology, Cambridge MA 02139
(7 October 1997)

The dynamical spin susceptibility χ''_π at wave vector (π,π) and the spectrum π'' of the spin-triplet particle–particle excitation with center of mass momentum (π,π) (π-excitation) are considered in the slave-boson formulation of the t–J-model. Propagators are calculated in a diagrammatic t-matrix approximation in the d-wave superconducting state for a wide doping range. The resulting spectra χ''_π and π'' both show a resonance at a doping dependent energy, in qualitative agreement with recent numerical cluster calculations. In underdoped systems, the peak position is comparable to that found in neutron scattering experiments. The peak in χ''_π as well as π'' is at low doping entirely caused by spin fluctuations, whereas the triplet particle–particle channel does not contribute as a collective mode.

The spin-triplet particle–particle excitation ('π-excitation')

$$\widehat{\pi}^\dagger = \sum_k (\cos(k_x) - \cos(k_y)) c^\dagger_{-k\uparrow} c^\dagger_{k+q\uparrow}$$

at wave vector $q = (\pi,\pi)$ has been introduced in [1] as a possible explanation for the '41 meV resonance' observed in neutron scattering on cuprates in the superconducting state (see e.g. [2,3]). It has been argued that $\widehat{\pi}^\dagger$ is an approximate collective eigenmode of the t–J or Hubbard model. The coupling of spin-triplet particle–particle excited states and spin-singlet particle–hole states in the superconducting phase then should lead to a resonance in the susceptibility $\chi''_\pi(\omega)$ at $q = (\pi,\pi)$ at the energy ω_0 of this π-mode.

We compare the susceptibility and the propagator of the π-excitation in a slave-boson theory for a wide range of hole concentrations (doping). Both calculated spectra χ''_π and π'' show a pronounced resonance at the same energy ω_0 , which is roughly given by the chemical potential μ as $\omega_0 \approx 2|\mu|$. The outcome is in qualitative agreement with the aforementioned prediction and with recent numerical [4,5] and diagrammatic calculations [6] . However, our interpretation differs from that originally envisioned in [1] : The diagrammatic spin-triplet particle–particle channel does not contribute as a collective mode to χ''_π or π'' . In underdoped systems not far from the transition to the Néel state, the resonance is solely caused by the 'RPA channel', which describes spin fluctuations mediated through spin-singlet particle–hole excitations of fermions.

The 'π-propagator' is given as

$$\pi(\omega) = \langle \mathcal{T}_\tau \, \widehat{\pi}(\tau) \widehat{\pi}^\dagger(\tau') \rangle^\omega \ . \qquad (1)$$

We start from the t–J-model and consider a Gutzwiller-projected π-propagator, Eq. (1) with $\widehat{\pi} \to P_G \widehat{\pi} P_G$. The calculations for $\pi(\omega)$ as well as the susceptibility $\chi_\pi(\omega)$ are performed within the standard slave-boson scheme. Diagrammatic expressions are based on a self-consistent perturbation theory with self energies taken at Hartree-Fock (mean-field) level. We consider the superconducting state at very low temperature, i.e., the d-wave pairing phase of fermions and fully condensed bosons. The t-matrix approximation for $\chi_\pi(\omega)$ and $\pi(\omega)$ are indicated in Figs. 1 and 2 respectively.

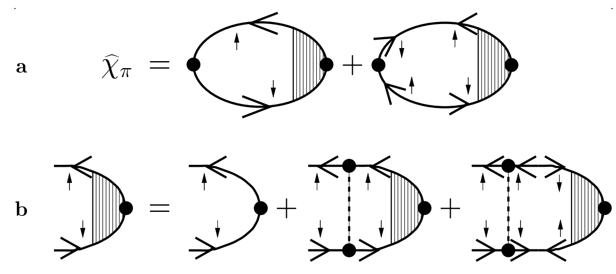

FIG. 1. **a:** Vertex renormalized mean-field susceptibility (part of the t-matrix approximation, see text). **b:** Vertex function for fermions in the d-wave pairing phase. The dashed line represents the nearest neighbor spin and density interaction $\sim J$ of the t–J-model.

The susceptibility is given by the vertex-renormalized mean-field bubbles displayed in Fig. 1a , which are to be inserted into

$$\chi_\pi(\omega) = \widehat{\chi}_\pi(\omega) / [1 - 2J \widehat{\chi}_\pi(\omega)] \ . \qquad (2)$$

Eq.(2) represents the particle–hole RPA channel (random phase approximation).

The single and double arrowed lines in Fig. 1 stand for the normal and pairing Green's functions of auxiliary fermions. The dashed line in Fig. 1b is the t–J-model's spin and density interaction for fermions on two nearest neighbor lattice sites i, j ,

$$J \sum_{<i,j>} [S_i S_j - \frac{1}{4} n_i n_j] \qquad (3)$$

with $n_i = \sum_\sigma f^\dagger_\sigma f_\sigma$.

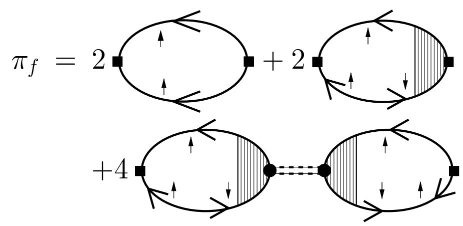

FIG. 2. t-matrix approximation for the π_f-propagator. The box indicates the phase factor $\cos(k_x) - \cos(k_y)$, k is the summed (loop) wave vector. The double dashed line stands for the effective interaction $\widetilde{J}(q,\omega)$ (see text). Prefactors count degenerate exchange parts.

The vertex corrections entering $\widehat{\chi}_\pi$ consist of the spin-singlet particle-hole (ph) ladder diagrams shown in Fig. 1b. The double arrowed (anomalous) Green's function introduces the ph channel in both time directions. In general it also allows for a coupling of the spin-triplet particle-particle (pp) channel into the singlet ph correlation function χ_π by transforming e.g. a spin-up fermion into a spin-down hole and vice versa. However, the pp channel would appear in χ_π as a vertex-function, involving at least one interaction vertex Eq. (3) with equal spin on both sites, which is zero [7]. This reflects the fact that Pauli's principle blocks any exchange process $\sim J = 4t^2/U$ for particles with equal spin in the Hubbard model. Thus the pp channel contributes no spectral weight to χ_π. This also holds if the pp channel is 'artificially' switched on by replacing $n_i n_j$ in Eq.(3) with $g\, n_i n_j$ and turning $g = 1 \to g = 0$: Recent numerical cluster calculations for the t–J-model [5] show that χ'' is not affected by varying the coefficient of the density–density interaction. In the following we stick to the case $g = 1$.

Numerical calculations in the t-matrix approximation are performed with mean-field parameters set to reflect a fermion bandwidth of $4J$ and a superconducting gap $\Delta_0 = 40\,\mathrm{meV} \approx 0.3J$. As has already been observed in earlier RPA calculations [8], an instability to the Néel state occurs at an unphysically high hole concentration (doping) x_c. Since the vertex corrections of the t-matrix approximation turn out to have no significant effect, we assume a further renormalization of $J \to \alpha J$ in Eq.(2). We have chosen $\alpha = 0.5$ such that x_c is reduced to ≈ 0.02.

Results for $\chi''_\pi(\omega)$ are shown in Fig. 3 (top) as continuous curves for several hole densities in the underdoped regime. The dominant feature is apparently a sharp and strongly doping dependent resonance. Its position ω_0 shifts from ≈ 0 at the magnetic instability ($x = x_c = 0.02$) to higher energies with increased doping, crossing the anticipated value $40\,\mathrm{meV} \approx 0.3J$ around $x = x_m = 0.12$. ω_0 is for $x > x_c$ roughly given

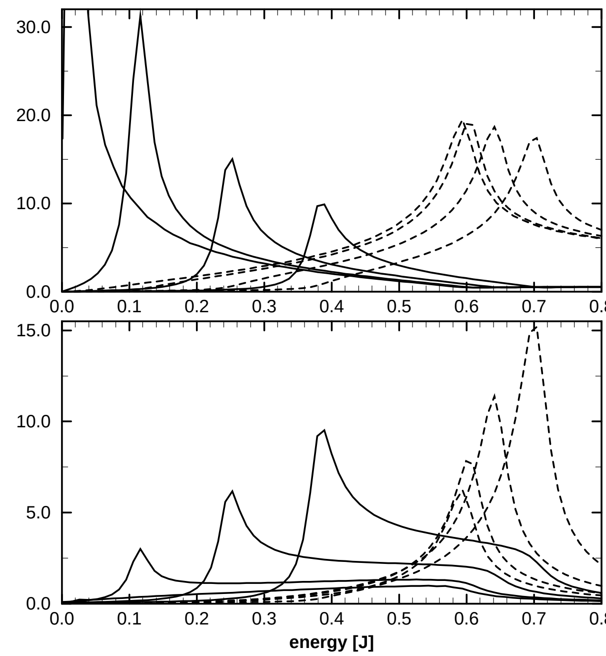

FIG. 3. **Top:** Susceptibility χ''_π in units of $(g\mu_B)^2/(2J)$ in the superconducting phase ($\Delta_0 = 0.3$) for hole concentrations $x = 0.02, 0.05, 0.1, 0.15$ fom left to right. Dashed curves are calculated from the bubble diagrams shown in Fig. 1a (multiplied by 10). Continuous curves result from the full t-matrix approximation, e.g., are calculated with the renormalization through the spin-fluctuation (RPA) channel Eq.(2) taken into account. **Bottom:** π_f-propagator in units of $1/J$ for the same set of x from left to right. Dashed lines result from the 1st and 2nd (bubble) diagram in Fig. 2. Continuous lines include the RPA channel (3rd diagram).

by the chemical potential μ as $\approx 2|\mu|$. This shift of the resonance with hole concentration is found in neutron scattering experiments on optimal [2,3] and underdoped YBCO-compounds [9,10]. The 'optimal' doping $x_m \approx 0.12$ found here also compares to experimental values. However, the spectral weight $\int d^2q\, \chi''(q,\omega) / \int d^2q$ comes out too small with respect to the experiment [11].

The resonance is caused by the spin-fluctuation RPA channel Eq.(2): For comparison, dashed curves in Fig. 3 (top) show the results for $\widehat{\chi}''_\pi(\omega)$, i.e., the renormalized bubble diagrams in Fig. 1a. The position of the doping dependent peak here is bound from below by $\approx 2\Delta_0 = 0.6J$, even for lowest doping. The contribution from the ph vertex corrections is quite small, $\widehat{\chi}''_\pi$ differs only slightly from the well known mean-field susceptibility.

The results for the susceptibility may be compared to the π-propagator Eq. (1). In slave-particle formulation, with bosons completely condensed at very low temperature, it reads $\pi(\omega) = x^2\, \pi_f(\omega)$. The prefactor x^2 is the (mean-field) probability of finding two empty lat-

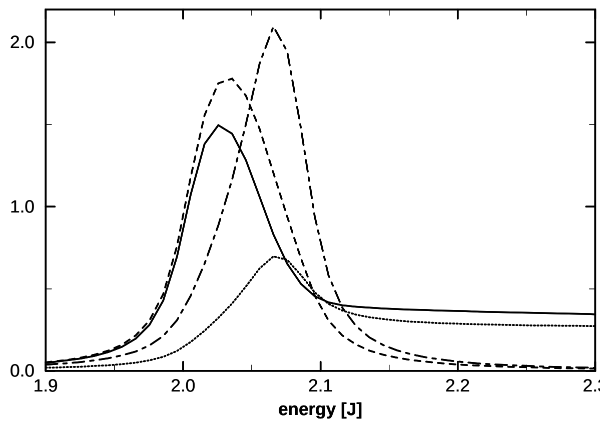

FIG. 4. Set of curves for a large chemical potential $\mu = -J$ in the superconducting state (see text). χ''_π and π''_f (scaled $\times 1/4$) are shown with the RPA-channel taken into account (continuous and dashed line respectively) and with the RPA channel omitted (dotted and dashed-dotted line resp.) .

tice sites when adding a spin-triplet pair of particles. The π-propagator for fermions $\pi_f(\omega)$ appearing here is formally identical to Eq. (1) , its t-matrix approximation is displayed in Fig. 2 . According to the discussion given above, the triplet *pp* channel may contribute only as the mean-field bubble (1st diagram). The singlet *ph* channel appears in vertex renormalizations in the 2nd and 3rd diagram. The 3rd diagram contains the contribution from the RPA channel via $\widetilde{J}(q,\omega)/2 = \frac{1}{2}J(q) + \frac{1}{4}J(q)\chi(q,\omega)J(q)$, indicated as a double dashed line in Fig. 2 .

The resulting spectrum $\pi''_f(\omega)$ in the underdoped regime is shown in Fig. 3 (bottom) for the same set of parameters and hole densities x as the susceptibility. Continuous lines correspond to the t-matrix approximation, dashed lines are calculated with the 3rd diagram in Fig. 2 (the coupling to the RPA channel) ignored. Again, the effect of the vertex corrections is negligible, the dashed curves differ only slightly from the mean-field theory (given by the 1st diagram in Fig. 2). Apparently π'' shows a pronounced peak which occurs at exactly the same position as the resonance in χ''_π , if the same approximation is used for both quantities. As has been pointed out, the spin-fluctuation (RPA) channel has to be taken into account in the underdoped regime $|\mu| < \Delta_0$, where the system is not far from the instability to the Néel state, and the RPA dominates χ''_π . In this case the peak in π'' is entirely caused by the coupling to spin fluctuations through $\widetilde{J}$. Note that its spectral weight decreases with reduced x , and vanishes at the transition to the Néel state ($x = x_c \approx 0.02$) .

The picture changes in a highly overdoped situation $|\mu| \gg \Delta_0$: Fig. 4 shows curves for a large chemical potential $\mu = -J$ (the breakdown of superconductivity in favor of the fermi-liquid state $\Delta_0 = 0$ is ignored for the moment). The peaks in χ''_π and π'' still occur at the same position $\approx 2|\mu|$, but the RPA induces only a slight shift, besides an enhancement of χ''_π . In the normal state $\Delta_0 = 0$ the resonance in χ''_π vanishes, whereas the peak in π'' remains as a delta function , $\pi''(\omega) \sim x^2\delta(\omega + 2\mu)$, as has also been observed in numerical calculations on highly doped clusters (referenced in [12]). In contrary to the low doping region, the highly overdoped regime $|\mu| \gg \Delta_0$ is well described by mean-field theory.

Acknowledgments: Discussions with W. Hanke and S.C. Zhang are gratefully acknowledged. One of the authors (JB) acknowledges a fellowship from the Deutsche Forschungsgemeinschaft, Germany.

[1] E. Demler and S. C. Zhang, Phys. Rev. Lett. **75**, 4126 (1995).
[2] H. F. Fong *et al.*, Phys. Rev. Lett. **75**, 316 (1995).
[3] P. Bourges, L. P. Regnault, L. Sidis, and C. Vettier, Phys. Rev. B **53**, 876 (1996).
[4] S. Meixner, W. Hanke, E. Demler, and S. C. Zhang, (1997), preprint (e-print `cond-mat/9701217`).
[5] R. Eder, W. Hanke, and S. C. Zhang, (1997), preprint (e-print `cond-mat/9707233`).
[6] S. C. Zhang, (1997), in preparation.
[7] G. Baskaran and P. W. Anderson, (1997), preprint (e-print `cond-mat/9706076`).
[8] H. Fukuyama, H. Kohno, and T. Tanamoto, J. Low Temp. Phys. **95**, 309 (1995).
[9] P. Dai *et al.*, Phys. Rev. Lett. **77**, 5425 (1996).
[10] H. F. Fong, B. Keimer, D. L. Milius, and I. A. Aksay, Phys. Rev. Lett. **78**, 713 (1997).
[11] P. Bourges *et al.*, (1997), preprint (e-print `cond-mat/9704073`).
[12] E. Demler, S. C. Zhang, S. Meixner, and W. Hanke, (1997), preprint (e-print `cond-mat/9705191`).